Generating adjoint expressions for Matlab

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Tenth European Workshop on Automatic Differentiation

Outline

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Extending our tool ADiMat with reverse mode

ADiMat implements AD *source transformation* of Matlab code.
Consider a function with signature **function** z = f(a)

- Forward mode: adimat f.m produces
  function [g_z, z] = g_f(g_a, a)
- Reverse mode: admproc f.m produces
  function [a_a, z] = a_f(a, a_z)
  via *XSL transformations*

In both cases the derivative variables can be either native doubles, which (in general) results in scalar mode or one can use one of several derivative classes, which allows vector mode.

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Adjoint code rules

Transformation rules found in the literature are for scalar valued variables

- Consider $z = e(x)$
- Adjoint statement: $\overline{x} \mathrel{+}= \frac{\partial e}{\partial x}\overline{z}$
- What happens when $e(x) = a * x * b$ and the variables are matrices?
- What is $\frac{\partial e}{\partial x}$ in this case?
- Dimensions of $\frac{\partial e}{\partial x}$ and $\overline{z}$ will not fit in general.

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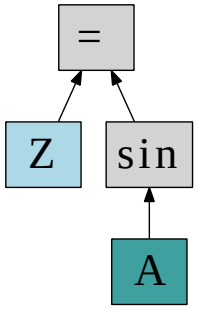
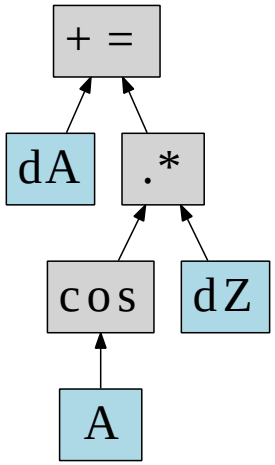
Adjoint rules: Sine

- Sine: $Z = sin(A)$



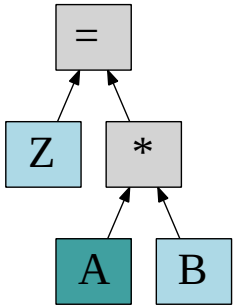
- $\overline{A} \mathrel{+}= \overline{Z} .* cos(A)$



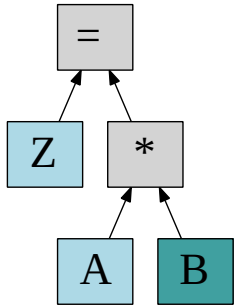
- Derivative variables have the same dimension as the variable they are associated with.
- Use upper case letters to indicate rule place holders.
- The place where $\mathrm{dZ} = \overline{Z}$ occurs is the *adjoint position*.

Adjoint rules: Multiplication

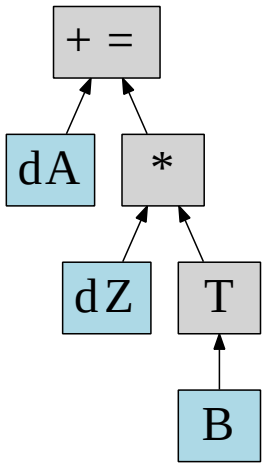
- Multiplication
  - $Z = A * B$, w.r.t. A



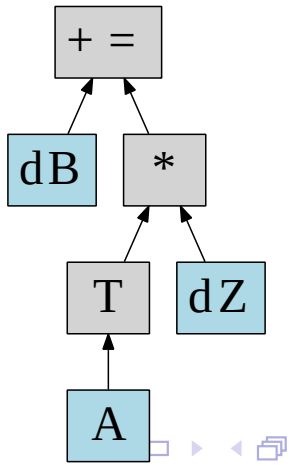
  - $Z = A * B$, w.r.t. B



  - $\overline{A} \mathrel{+}= \overline{Z} * B^T$



  - $\overline{B} \mathrel{+}= A^T * \overline{Z}$

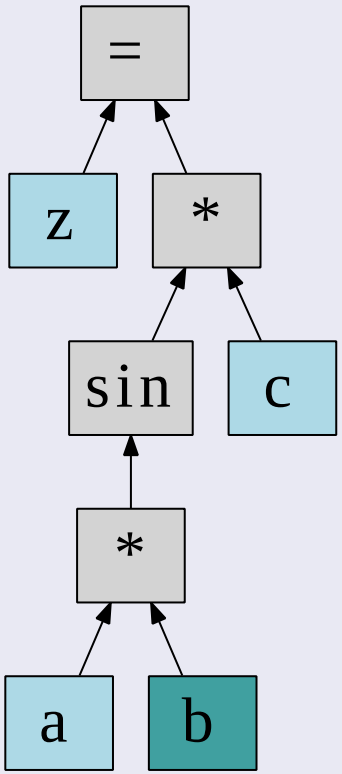


Outline

Example statement

- Consider the statement: $z = \sin(a * b) * c$

Syntax tree

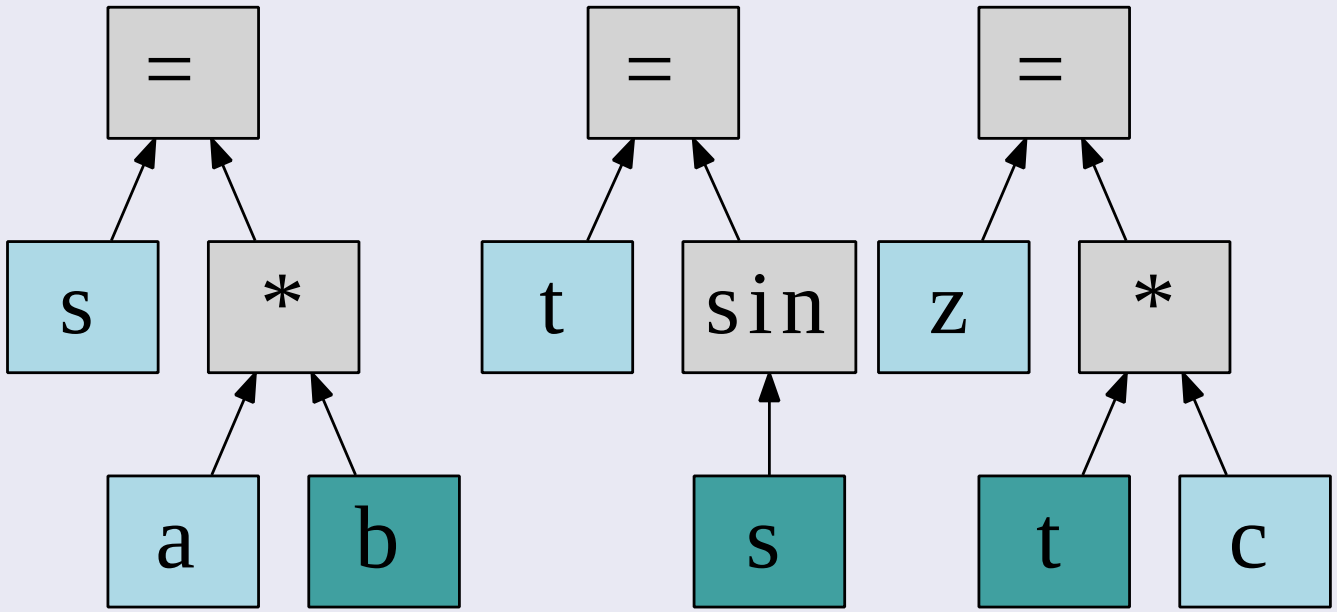


Outline

Canonicalized statement

- Canonicalization: $s = a * b$, $t = \sin(s)$, $z = t * c$

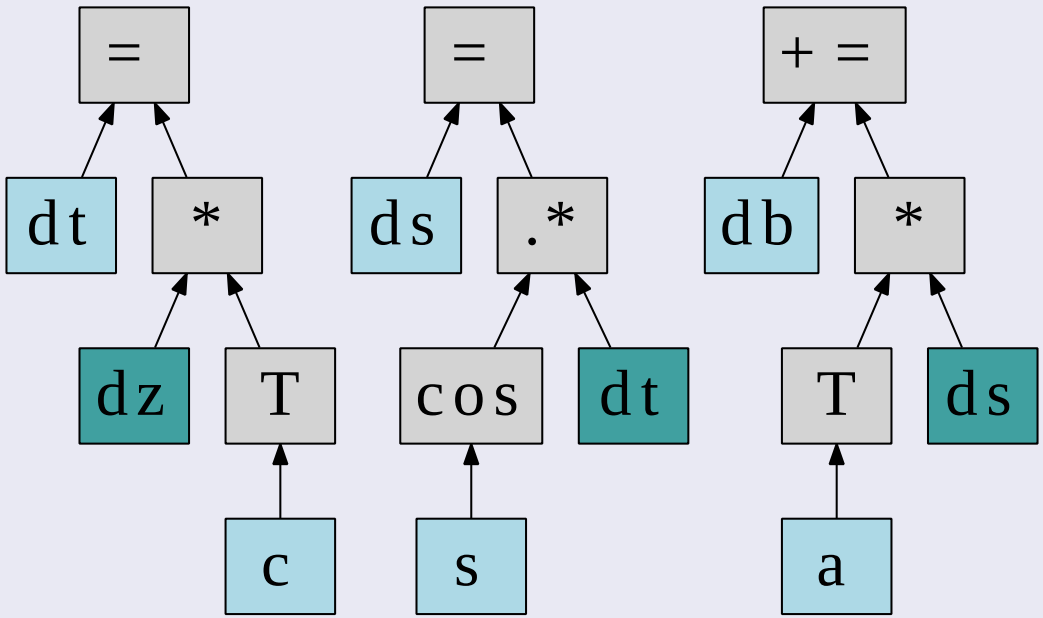
Syntax trees



Adjoint canonicalized statements

- Reverse adjoint statements:
  $\bar{t} = \bar{z} * c^T, \bar{s} = \cos(s) .* \bar{t}, \bar{b} \mathrel{+}= a^T * \bar{s}$

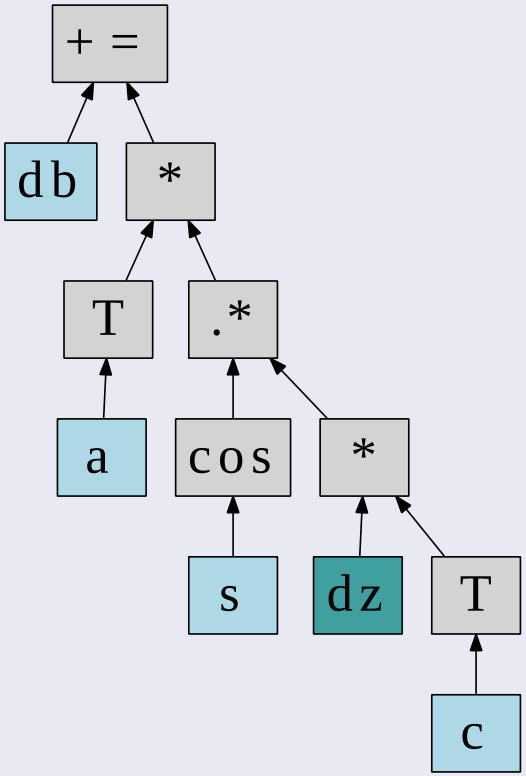
Syntax trees



Putting it back together

- Single adjoint statement: $\overline{b} \mathrel{+}= a^T * (\cos(a * b) .* (\overline{z} * c^T))$

Merged syntax tree



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Observations

- The outermost $*$-operator has the adjoint of the statement LHS at the adjoint position.
- The second level operator sin has at the adjoint position the expression sub-tree that was produced by the outermost operator.
- The evalation order is inverted.

Recursive procedure

- Consider a statement $z = e$, assigning expression $e(x)$ to z. What is the adjoint expression w.r.t. x for that statement.
- Let $a_1 = \text{adjexp}(e, a_0)$ be the adjoint expression of the outermost operation in expression e, where $a_0 = \overline{z}$.
- Then, $a_2 = \text{adjexp}(\text{active-child}(e), a_1)$ is the adjoint expression of the second level operator, where active-child selects the child of the top along the path to variable x.
- Finally, a_k is the adjoint of the expression e w.r.t. variable x, where k is the depth of x in e.

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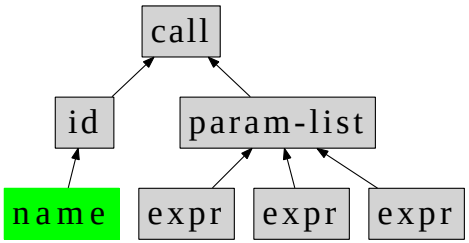
Recursive template calls

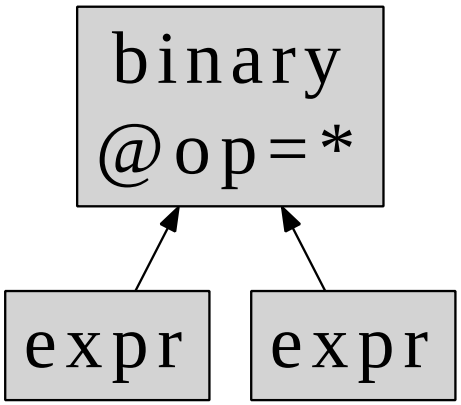
- Traverse the expression tree in top down order with apply-template
- Pass along two parameters
  - wrt – id of variable node in the expression
  - adj – adjoint constructed so far
- xsl:apply−templates to that child which has the node with id $wrt among its descendant−or−self::.
  - wrt – $wrt
  - adj – new expression according to rule for current node, inserting $adj at the adjoint position of the rule

Template For Sine



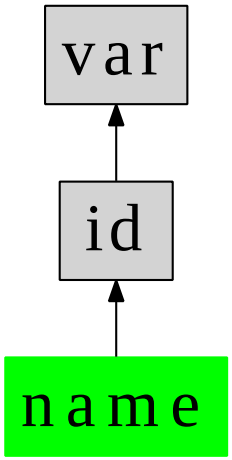

```
<xsl:template match="call[id = 'sin']" mode="diff">
  <xsl:param name="wrt"/>
  <xsl:param name="adj"/>
  <xsl:apply-templates select="*[2]/*" mode="diff">
    <xsl:with-param name="wrt" select="$wrt"/>
    <xsl:with-param name="adj">
      <binary op=".*">
        <call>
          <id>cos</id>
          <xsl:apply-templates select="*[2]"/>
        </call>
        <xsl:copy-of select="$adj"/>
      </binary>
    </xsl:with-param>
  </xsl:apply-templates>
</xsl:template>
```

Template For Multiplication




```
<xsl:template match="binary[@op = '*']" mode="diff">
  <xsl:param name="wrt"/>
  <xsl:param name="adj"/>
  <xsl:variable name="which"
    select="*[descendant-or-self::*[generate-id(.) = $wrt]]"/>
  <xsl:apply-templates select="$which" mode="diff">
    <xsl:with-param name="wrt" select="$wrt"/>
    <xsl:with-param name="adj">
      <xsl:choose>
        <xsl:when test="count($which/following-sibling::*)">
          <adjoint-left-multiplication>
            <xsl:copy-of select="$which"/>
            <xsl:copy-of select="$adj"/>
            <xsl:copy-of select="*[2]"/>
          </adjoint-left-multiplication>
        </xsl:when>
        <xsl:otherwise>
          <!-- ... -->
        </xsl:otherwise>
      </xsl:choose>
    </xsl:with-param>
  </xsl:apply-templates>
</xsl:template>
```

Template For Variable Nodes




```
<xsl:template match="var" mode="diff">
  <xsl:param name="wrt"/>
  <xsl:param name="adj"/>
  <xsl:choose>
    <xsl:when test="generate-id() = $wrt">
      <xsl:copy-of select="$adj"/>
    </xsl:when>
    <xsl:otherwise>
      <literal>0</literal>
    </xsl:otherwise>
  </xsl:choose>
</xsl:template>
```

Template For Statement

```
<xsl:template match="binary[@op = '=']" mode="adjoint">
  <!-- pop variables, ... -->
  <xsl:apply-templates mode="adjoint-assignment"
      select="*[2]/descendant-or-self::var">
    <xsl:with-param name="this" select="."/>
  </xsl:apply-templates>
  <!-- zero adjoint of variable written, ... -->
</xsl:template>

<xsl:template match="var" mode="adjoint-assignment">
  <xsl:param name="this"/>
  <xsl:param name="adj">
    <xsl:apply-templates select="ancestor::binary[@op = '='][1]/*[1]"
                         mode="adjoint-var-of-statement"/>
  </xsl:param>
  <xsl:variable name="myid" select="generate-id()"/>
  <adjoint-increment>
    <target>
      <xsl:apply-templates select="(parent::array|.)[1]"/>
    </target>
    <incr>
      <xsl:apply-templates select="$this/*[2]" mode="diff">
        <xsl:with-param name="wrt" select="generate-id(.)"/>
        <xsl:with-param name="adj" select="$adj"/>
      </xsl:apply-templates>
    </incr>
  </adjoint-increment>
</xsl:template>
```

Outline

Example: A Times B Times C

```
function z = mult3(a, b, c)
   z = a * b * c;
end
```

```
function [a_a, a_b, a_c, nr_z] = a_mult3(a, b, c, a_z)
   z = a * b * c;
   nr_z = z;
   [a_a a_b a_c] = a_zeros(a, b, c);
   a_a = a_a + a_z*(b * c).';
   a_b = a_b + a.'*a_z*c.';
   a_c = a_c + b.'*a.'*a_z;
end
```

admproc −s adjoint−reductions='no' −−nocanonicalize mult3.m

Outline

Conclusion

- Adjoints of arbitrarily nested expressions
- Ability to turn off code canonicalization
- Ability to generate code for only scalars or only matrices
- Simple implementation in XSLT

Outlook

- Represent derivative rules in one format for both forward and reverse?
- Handle cases where adjoints are given by algorithm, not an expression